

Thermodynamics of lattice QCD with 3 flavours of colour-sextet quarks II: $N_t = 6$ and $N_t = 8$.

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We have been studying QCD with 2 flavours of colour-sextet quarks as a candidate walking-Technicolor theory using lattice-QCD simulations. The evolution of the coupling constant with lattice spacing is measured at the finite-temperature chiral transition to determine if this theory is asymptotically free and hence QCD-like. The lattice spacing is varied by changing the number of lattice sites, N_t , in the Euclidean time direction. QCD with 3 flavours is studied for comparison. Since this theory is expected to be conformal, with an infrared fixed point, the coupling constant at the chiral transition should approach a non-zero value as N_t becomes large. Our earlier simulations on lattices with $N_t = 4$ and $N_t = 6$ exhibited a significant decrease in coupling at the chiral transition as N_t was increased. We have now extended these simulations to $N_t = 8$, and performed additional simulations at $N_t = 6$ to measure the coupling constant at the chiral transition more precisely. These indicate that while there is an appreciable decrease in coupling between $N_t = 6$ and $N_t = 8$, this is much smaller than that between $N_t = 4$ and $N_t = 6$. Thus we are hopeful that we are approaching the large- N_t limit. However, further simulations at larger N_t (s) are needed.

I. INTRODUCTION

The LHC has demonstrated its ability to probe the Higgs sector of the Standard Model. This has revived interest in trying to understand this sector in more detail. It is understood that the original description of this part of the standard model in terms of an elementary scalar field is at best an effective field theory. We are interested in studying models where the Higgs field is composite. The most promising of these are the Technicolor theories [1, 2], Yang-Mills gauge theories with massless fermions whose Goldstone (techni-)pions play the role of the Higgs field giving masses to the W^\pm and Z . It has been observed that phenomenological difficulties with Technicolor theories which are simply scaled-up QCD can be avoided if the fermion content is chosen such that there is a range of mass scales over which the gauge coupling evolves very slowly – ‘walks’ [3–6].

For a chosen gauge group and N_f fermions in a chosen representation, there is typically a value of N_f below which the one- and two-loop terms in β , which describes the evolution of the coupling are both negative, and the theory is asymptotically free and probably also confining with spontaneously broken chiral symmetry (QCD-like). For N_f large enough both terms are positive, and asymptotic freedom is lost. In between these regimes is a range of N_f s for which the 1-loop term is negative and the 2-loop term is positive. Theories in this regime are still asymptotically free, but if this two-loop β is a good guide to its behaviour, there is a second, infrared-attractive fixed point, and the theory is conformal. However, if before this would-be IR fixed point is reached, the coupling becomes strong enough that a chiral condensate forms, this fixed point is avoided and the theory is confining. Because of the nearby IR fixed point, there will be a range of mass scales over which the coupling evolves very slowly, and the theory walks. For an extensive discussion of this behaviour for $SU(N)$ gauge theories and a guide to the earlier literature, see for example [7]. Such behaviour is clearly non-perturbative, and lends itself to study using simulation methods developed for lattice QCD.

We [8–10], along with others [11–22], have been studying (techni)-QCD with 2 flavours of (techni)-colour-sextet (techni)-quarks, which is a candidate walking-Technicolor theory. For the rest of the paper we will drop the prefix ‘techni’ and remember that we are dealing not with normal QCD, but with a scaled-up version where $f_\pi \approx 246$ GeV, rather than ≈ 93 MeV. For QCD with colour-sextet quarks, the 3-flavour theory is also in the regime where the 1-

and 2-loop contributions have opposite sign. 3 flavours is so close to the number ($3\frac{3}{10}$) above which asymptotic freedom is lost, that the non-trivial zero of the 2-loop β -function is at a small enough value of $\alpha_s = g^2/4\pi$ (≈ 0.085), that it is unlikely that a chiral condensate is formed before it is reached. Thus it is believed that this theory will have an infrared fixed point at a value close to that predicted perturbatively, and so for massless quarks, it will be conformal. We therefore find it useful to study QCD with 3 colour-sextet quarks for comparison with QCD with 2 colour-sextet quarks, to see if they do indeed behave rather differently. In fact non-lattice methods, which attempt to determine the walking and conformal windows, place the critical number of flavours for QCD with colour-sextet quarks closer to 2 [7, 23–28].

We simulate lattice QCD with 3 flavours of light colour-sextet staggered quarks at finite temperatures using the RHMC method [29] to tune to 3 flavours. The simple Wilson plaquette action is used for the gauge fields. Finite temperature is achieved by simulating on a lattice whose spatial extent N_s is infinite and whose temporal extent N_t is finite. In practice, N_s is also finite, but $N_s \gg N_t$. The temperature is then $T = 1/N_t a$ where a is the lattice spacing. If T is fixed at a finite temperature phase transition, then $a \rightarrow 0$ as $N_t \rightarrow \infty$. We work with the chiral-symmetry restoration transition (which means that we need to extrapolate to zero quark mass). If this is indeed a finite temperature transition, the coupling constant at this transition will approach zero as $N_t \rightarrow \infty$ in a manner described by asymptotic freedom. In the case where the continuum theory is conformal and chiral symmetry is unbroken in the continuum limit, chiral symmetry is restored at a bulk transition, where the coupling constant is finite and independent of N_t if N_t is sufficiently large.

Our earlier simulations of the 3-flavour theory were performed at $N_t = 4$ and 6 [30]. Between $N_t = 4$ and 6, the value of $\beta = 6/g^2$ at the chiral transition (β_χ) showed a relatively large increase (~ 0.3). This we interpreted as being because it occurs at a coupling which is strong enough that the fermions are bound into a chiral condensate and do not contribute significantly to the evolution of the coupling constant. The theory is effectively a pure gauge theory, and what is observed is the finite-temperature chiral transition of the quenched theory where coupling-constant evolution is that of 0-flavour QCD. We have now extended our simulations to $N_t = 8$. (Preliminary results were presented at Lattice 2012 and Lattice 2013 [10].) In addition we have had to extend our $N_t = 6$ simulations to use more β values close to the chiral transition. Between $N_t = 6$ and 8 β_χ increases by ~ 0.1 which is small

enough to indicate that its evolution is no longer controlled by quenched dynamics, however, it does not yet indicate that the coupling is approaching a finite constant. Thus larger N_t s are called for.

In section 2 we give some technical details. Section 3 describes the simulations and results. Discussions and conclusions are given in section 4.

II. TECHNICAL DETAILS

We use the unimproved Wilson (plaquette) action for the gauge fields:

$$S_g = \beta \sum_{\square} \left[1 - \frac{1}{3} \text{Re}(\text{Tr} U U U U) \right]. \quad (1)$$

The unimproved staggered-fermion action is used for the sextet quarks:

$$S_f = \sum_{\text{sites}} \left[\sum_{f=1}^{N_f/4} \psi_f^\dagger [\not{D} + m] \psi_f \right], \quad (2)$$

where $\not{D} = \sum_{\mu} \eta_{\mu} D_{\mu}$ with

$$D_{\mu} \psi(x) = \frac{1}{2} [U_{\mu}^{(6)}(x) \psi(x + \hat{\mu}) - U_{\mu}^{(6)\dagger}(x - \hat{\mu}) \psi(x - \hat{\mu})]. \quad (3)$$

Here $U^{(6)}$ is the sextet representation of U , i.e. the symmetric part of the tensor product $U \otimes U$. When N_f is not a multiple of 4 we use the fermion action:

$$S_f = \sum_{\text{sites}} \chi^\dagger \{ [\not{D} + m] [-\not{D} + m] \}^{N_f/8} \chi. \quad (4)$$

The operator which is raised to a fractional power is positive definite and we choose the real positive root. This yields a well-defined operator. We assume that this defines a sensible field theory in the zero lattice-spacing limit, ignoring the rooting controversy. (See for example [31] for a review and guide to the literature on rooting.) What is important for comparison with the 2-flavour theory is that this action differs only in the value of N_f from the action used in those simulations.

We simulate using the Rational Hybrid Monte Carlo (RHMC) algorithm, in which the fractional powers of the quadratic Dirac operator are approximated by an optimal (diagonal) rational approximation, to the required precision. A global Metropolis accept/reject step at the end of each trajectory removes errors due to discretization of molecular-dynamics time, associated with updating the fields.

If the massless theory is QCD-like – confining with spontaneously broken chiral symmetry – in the continuum limit, the chiral phase transition and the deconfinement transition (to the extent that it is well-defined) will be finite temperature transitions occurring at fixed temperatures T_χ and T_d respectively. At small enough lattice spacing – large enough N_t – the evolution of the lattice coupling constants will be governed by the Callan-Symanzik β -function. To 2-loops:

$$\beta(g) = -b_1 g^3 - b_2 g^5. \quad (5)$$

Expressing our coupling constant evolution in terms of $\beta = 6/g^2$ (We apologize for the fact that we are using β for 2 different purposes)

$$\Delta\beta(\beta) = \beta(a) - \beta(\lambda a) = (12b_1 + 72b_2/\beta) \ln(\lambda) \quad (6)$$

to this order in g . For N_f flavours of sextet quarks,

$$\begin{aligned} b_1 &= \left(11 - \frac{10}{3}N_f\right) / 16\pi^2 \\ b_2 &= \left(102 - \frac{250}{3}N_f\right) / (16\pi^2)^2. \end{aligned} \quad (7)$$

To this order the second zero of β , the one associated with an IR fixed point occurs at $g = g_c$, where:

$$g_c^2 = -b_1/b_2 \quad (8)$$

For $N_f = 3$, this gives

$$g_c^2 = 4\pi^2/37 \approx 1.067, \quad (9)$$

and thus

$$\alpha_s = g_c^2/(4\pi) \approx 0.0849. \quad (10)$$

At this coupling the lattice quantity

$$\beta = \beta_c = 6/g_c^2 \approx 5.623. \quad (11)$$

Note that to this order, the β -function has the same coefficients independent of renormalization scheme, and whether we are referring to a ‘bare’ or to a ‘renormalized’ coupling. So, this zero also occurs at the same value, independent of scheme.

Since these two-loop calculations indicate that the running coupling does not get very large before the infrared fixed point is reached, it would be surprising if a condensate formed

to enable this fixed point to be avoided. We contrast this with the 2-flavour case, where g_c^2 and hence α_s is an order of magnitude larger than for the 3-flavour theory. Approximate calculations and arguments support the idea that QCD with 3 sextet quarks is conformal [7, 23–28]

The values of β_d at $N_t = 4$ and 6 are much smaller than those of β_χ at the same N_t s. Since we have concluded that the chiral transition for these N_t values lies in the strong-coupling regime where coupling constant evolution is described by quenched dynamics, the deconfinement transition lies at even stronger couplings and is unlikely to emerge until much larger N_t . In fact, β_d lies considerably below β_c at these N_t s, a region inaccessible to 2-loop perturbation theory. We therefore concentrate our efforts on the evolution of the coupling constant at the chiral transition.

Although the chiral condensate, measured in our simulations, shows evidence that it will vanish in the chiral limit for sufficiently large β , its β dependence for the quark masses we use is too smooth to enable an accurate determination of β_χ . This is still true when we use the method of the Lattice Higgs Collaboration [18] to remove much of the a^{-2} divergence from the lattice quantity. We therefore use the position of the peak in the chiral susceptibility extrapolated to $m = 0$ as our estimate of β_c . The chiral susceptibility is given by

$$\chi_{\bar{\psi}\psi} = V \left[\langle (\bar{\psi}\psi)^2 \rangle - \langle \bar{\psi}\psi \rangle^2 \right] \quad (12)$$

where the $\langle \rangle$ indicates an average over the ensemble of gauge configurations and V is the space-time volume of the lattice. Since the fermion functional integrals have already been performed at this stage, this quantity is actually the disconnected part of the chiral susceptibility. Since we use stochastic estimators for $\bar{\psi}\psi$, we obtain an unbiased estimator for this quantity by using several independent estimates for each configuration (5, in fact). Our estimate of $(\bar{\psi}\psi)^2$ is then given by the average of the (10) estimates which are ‘off diagonal’ in the noise.

III. SIMULATIONS OF LATTICE QCD WITH 3 SEXTET QUARKS.

A. $N_t = 6$

We simulate lattice QCD with 3 flavours of colour-sextet quarks on a $12^3 \times 6$ lattice, using quark masses $m = 0.02$, $m = 0.01$ and $m = 0.005$ which should be adequate to

enable extrapolation to the chiral limit. Because we are primarily interested in the chiral transition we concentrate on the range $5.5 \leq \beta \leq 7.0$. Our earlier simulations covered this range with β values spaced by 0.1, using 10,000 length-1 trajectories for each (β, m) . Since we have determined that $\beta_\chi(N_t = 8) - \beta_\chi(N_t = 6) \sim 0.1$ this spacing is inadequate to determine this evolution of the coupling at the chiral transition with any precision. We have therefore extended our simulations at the lowest quark mass (0.005), to cover the interval $6.2 \leq \beta \leq 6.4$, which is close to this transition, with β s spaced by 0.02. In addition, we have increased our statistics to 100,000 trajectories at each of these β s. Note that we are only dealing with the phase with a real positive Wilson Line (Polyakov Loop).

Figure 1 shows the chiral condensates ($\langle \bar{\psi}\psi \rangle$) as functions of β from these simulations. $\langle \bar{\psi}\psi \rangle$ is normalized to one staggered fermion (4 continuum flavours). Note also that these are lattice regularized quantities. No attempt has been made to subtract the quadratic divergence at $m \neq 0$. Although these imply that $\langle \bar{\psi}\psi \rangle$ will vanish in the chiral limit for sufficiently large β , the dependence on β is too smooth to obtain β_χ , the position of the phase transition at which this vanishing occurs.

For this reason, we measure the disconnected chiral susceptibility, defined in equation 12, to determine β_χ . In the chiral limit, this quantity diverges at $\beta = \beta_\chi$. For finite m this susceptibility has a peak, which becomes more pronounced and approaches β_χ , as $m \rightarrow 0$. In practice we have found that the position of the peak β_{max} has little m dependence, and so β_{max} for the smallest m should be a good estimate of β_χ . We use 5 stochastic estimators of $\langle \bar{\psi}\psi \rangle$ at the end of each trajectory, to obtain an unbiased estimator for $\chi_{\bar{\psi}\psi}$.

Figure 2 shows the susceptibilities measured during these simulations. The peak in the $m = 0.005$ susceptibility is very pronounced, that for the two higher masses somewhat less so. However, it is clear that the position of the peak (β_{max}) has little m dependence. We tried using Ferrenberg-Swendsen reweighting to obtain precise estimates for the value of β_{max} . However, despite the fact that the β values in the transition region are sufficiently close that there is significant overlap between plaquette distributions for neighbouring β s, we had little success. Therefore, to make maximal use of our data, we fit the susceptibilities for β values close to the peak to a parabola, namely:

$$\chi_{\bar{\psi}\psi} = a - b(\beta - \beta_{max})^2 \quad (13)$$

For $m = 0.005$, a fit over the range $6.2 \leq \beta \leq 6.4$ yielded $\beta_{max} = 6.278(2)$ with $\chi^2/d.o.f =$

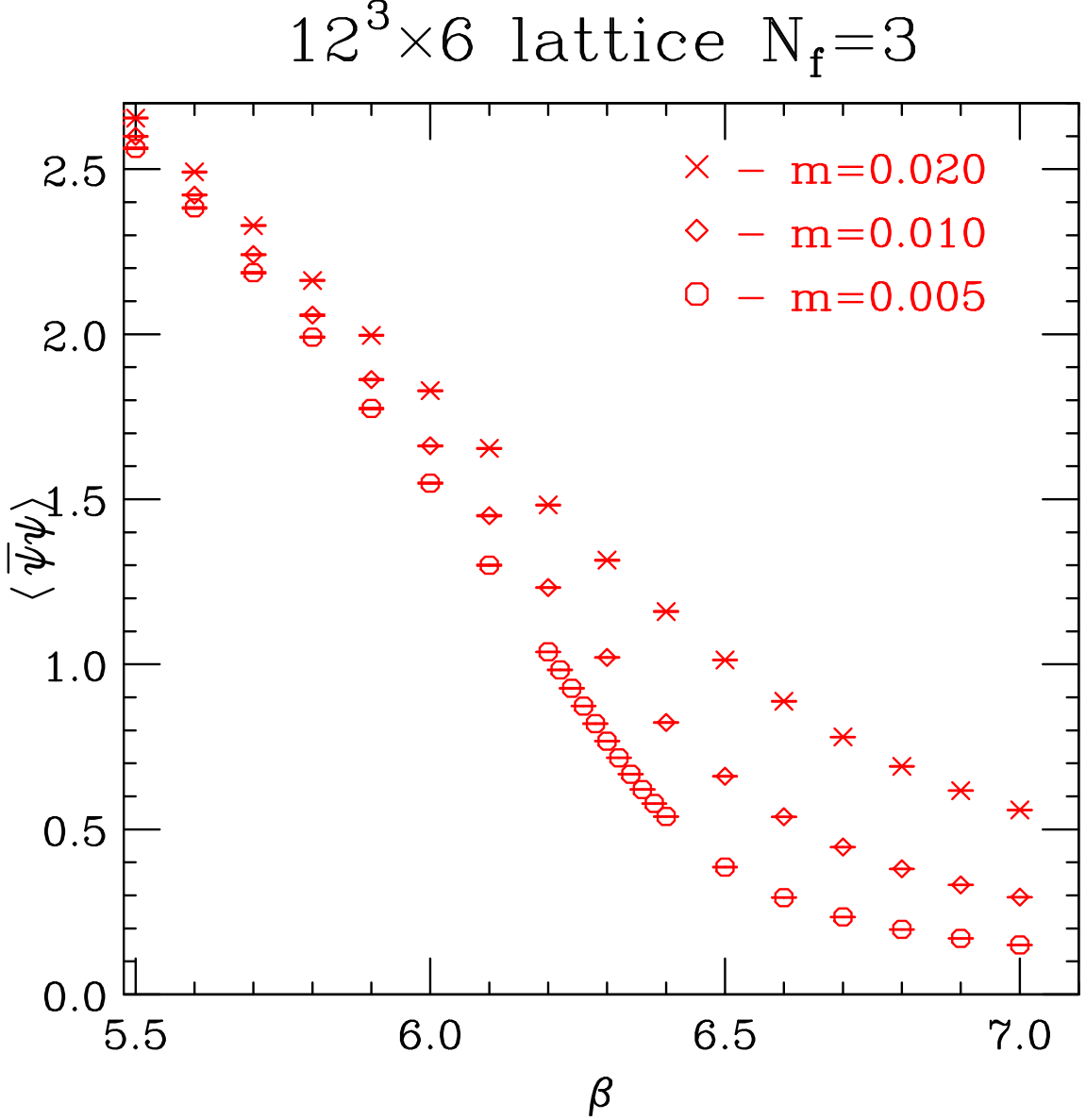


FIG. 1: $\langle \bar{\psi}\psi \rangle$ as functions of $\beta = 6/g^2$ on a $12^3 \times 6$ lattice, in the state with a real positive Wilson Line, for $m = 0.02, 0.01, 0.005$.

0.85. This fit is shown in figure 3. It is stable on removal of the point at $\beta = 6.2$ or that at $\beta = 6.4$ from our fit. We also performed fits to our $m = 0.01$ and $m = 0.02$ ‘data’. Since the measurements used in these fits are spaced by 0.1 in β and the peaks are broad and less pronounced, we expect these fits to be less reliable than those for $m = 0.005$. For $m = 0.01$, a fit over $6.0 \leq \beta \leq 6.5$ yields $\beta_{max} = 6.261(8)$ with $\chi^2/d.o.f = 2.1$ while a fit over $6.1 \leq \beta \leq 6.5$ yields $\beta_{max} = 6.278(9)$ with $\chi^2/d.o.f = 1.2$. Finally for $m = 0.02$, a fit over $5.9 \leq \beta \leq 6.6$ gives $\beta_{max} = 6.286(8)$ with $\chi^2/d.o.f = 0.63$, while one over $6.0 \leq \beta \leq 6.6$

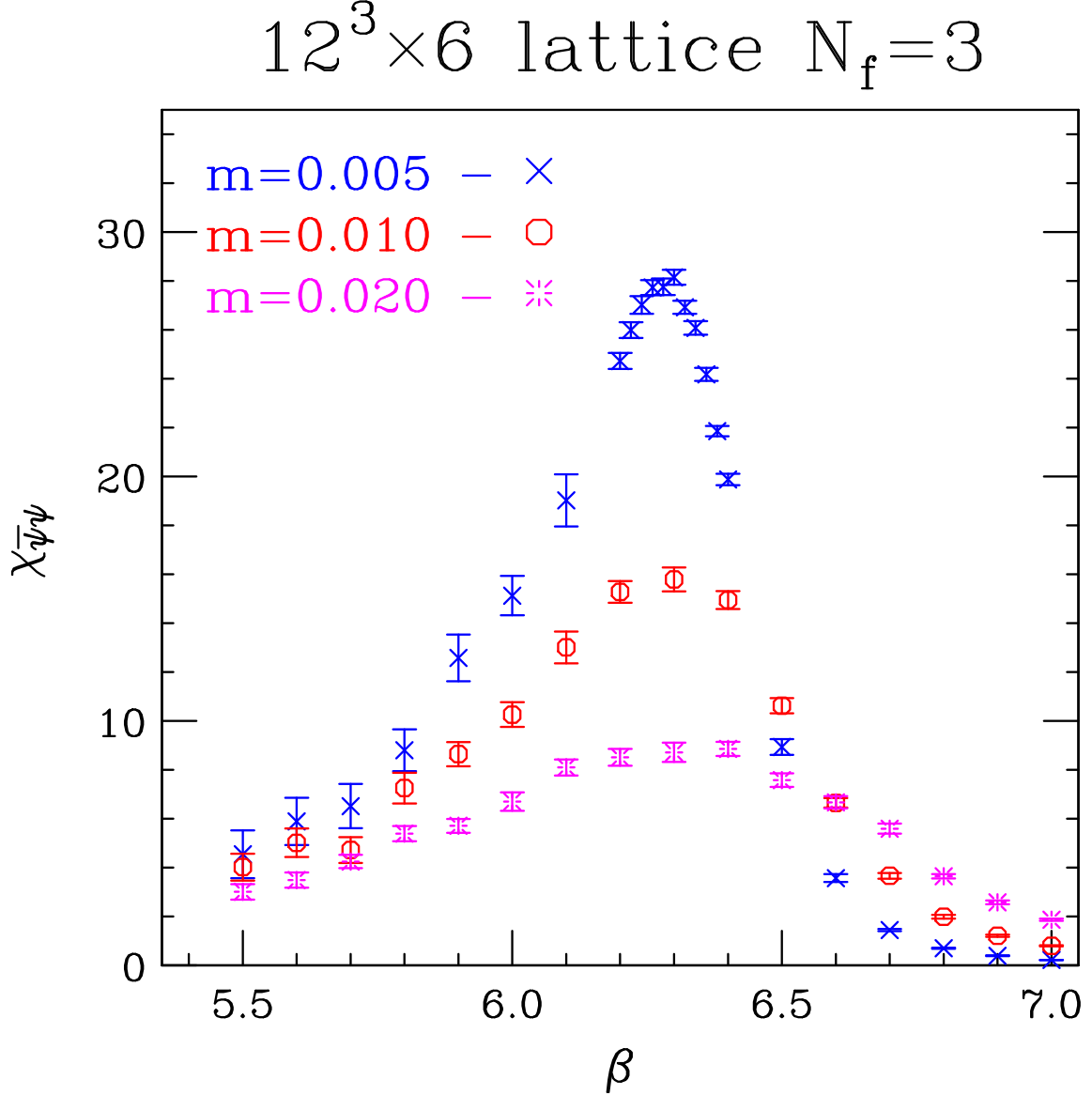


FIG. 2: Chiral susceptibilities as functions of $\beta = 6/g^2$ on a $12^3 \times 6$ lattice, in the state with a real positive Wilson Line, for $m = 0.02, 0.01, 0.005$.

gives $\beta_{max} = 6.294(10)$ with $\chi^2/d.o.f = 0.57$. Thus we see that the position of the peak is almost independent of m which justifies taking the $m = 0.005$ value of β_{max} as β_χ .

B. $N_t = 8$

We perform simulations on $16^3 \times 8$ lattices at $m = 0.01$ and $m = 0.005$. For $m = 0.01$ we simulate for β s in the range $5.4 \leq \beta \leq 7.0$ at intervals of 0.1 in β , using runs of

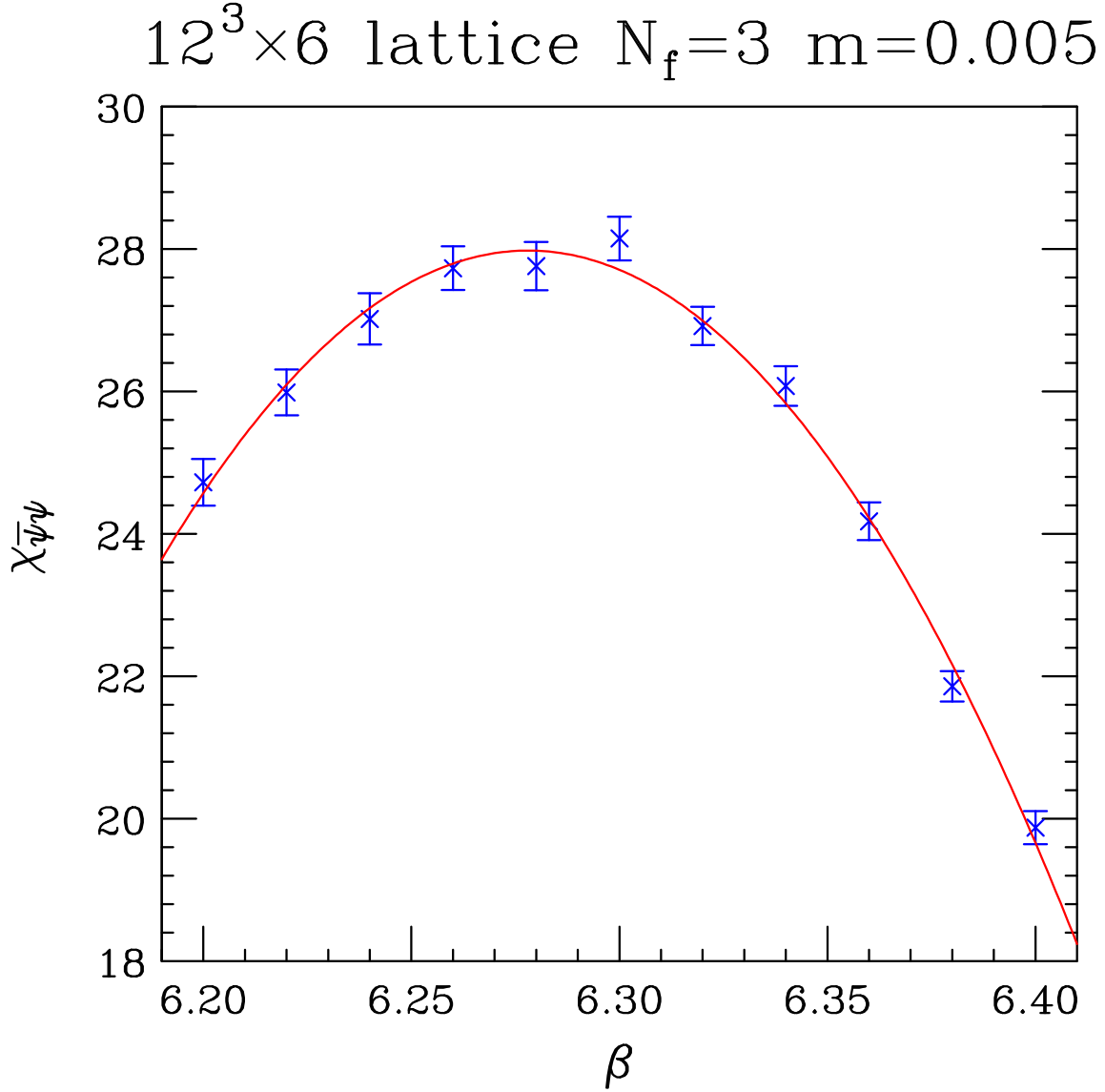


FIG. 3: Chiral susceptibility for $m = 0.005$ as a function of β on a $12^3 \times 6$ lattice, showing the fit to a parabola mentioned in the text.

10,000 trajectories at each β . For $m = 0.005$ we perform simulations for β s in the range $5.8 \leq \beta \leq 7.0$, again at β separations of 0.1 with 10,000 trajectories at each β , except in the range $6.28 \leq \beta \leq 6.5$, where we simulate at β s spaced by 0.02 with 100,000 trajectories for each β .

Figure 4 shows the chiral condensates measured in these simulations. Part a is the unsubtracted condensate, while part b is the same condensates after subtracting much of the quadratic divergence of the unsubtracted condensate using the method favoured by the

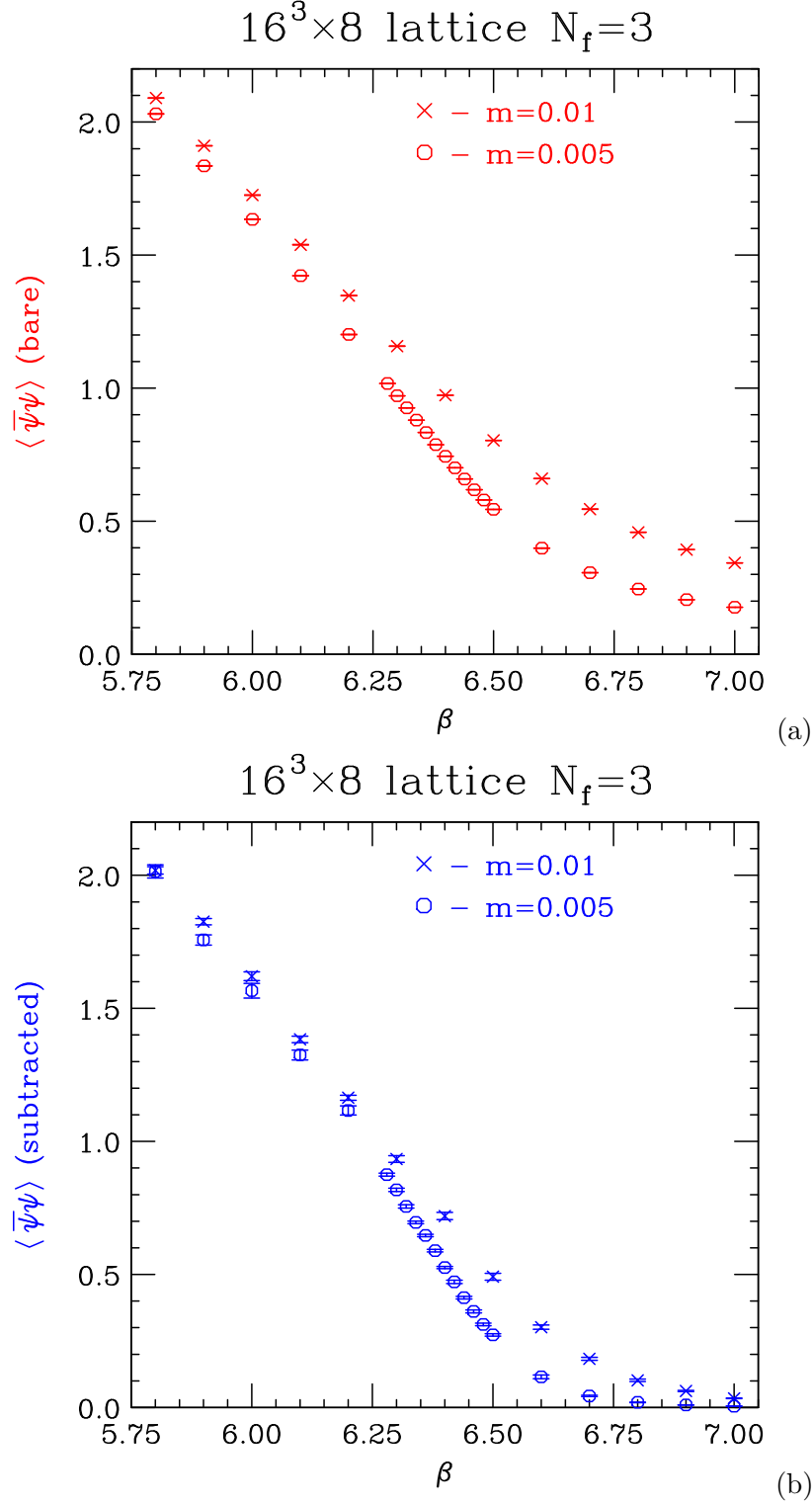


FIG. 4: a) $\langle \bar{\psi}\psi \rangle$ as functions of $\beta = 6/g^2$ on a $16^3 \times 8$ lattice, in the state with a real positive Wilson Line, for $m = 0.01, 0.005$.

b) $\langle \bar{\psi}\psi \rangle$ on a $16^3 \times 8$ lattice, subtracted using the valence subtraction used by the Lattice Higgs Collaboration.

Lattice Higgs Collaboration.

$$\langle \bar{\psi}\psi \rangle_{sub} = \langle \bar{\psi}\psi \rangle - \left(m_V \frac{\partial}{\partial m_V} \langle \bar{\psi}\psi \rangle \right)_{m_V=m} \quad (14)$$

where m_V is the valence quark mass. Although the subtracted condensate indicates that it will vanish in the chiral limit for large enough β , more clearly than the unsubtracted condensate, it still does not yield a precise estimate of β_χ . Hence we again turn to the chiral susceptibility to obtain an accurate estimate of β_χ .

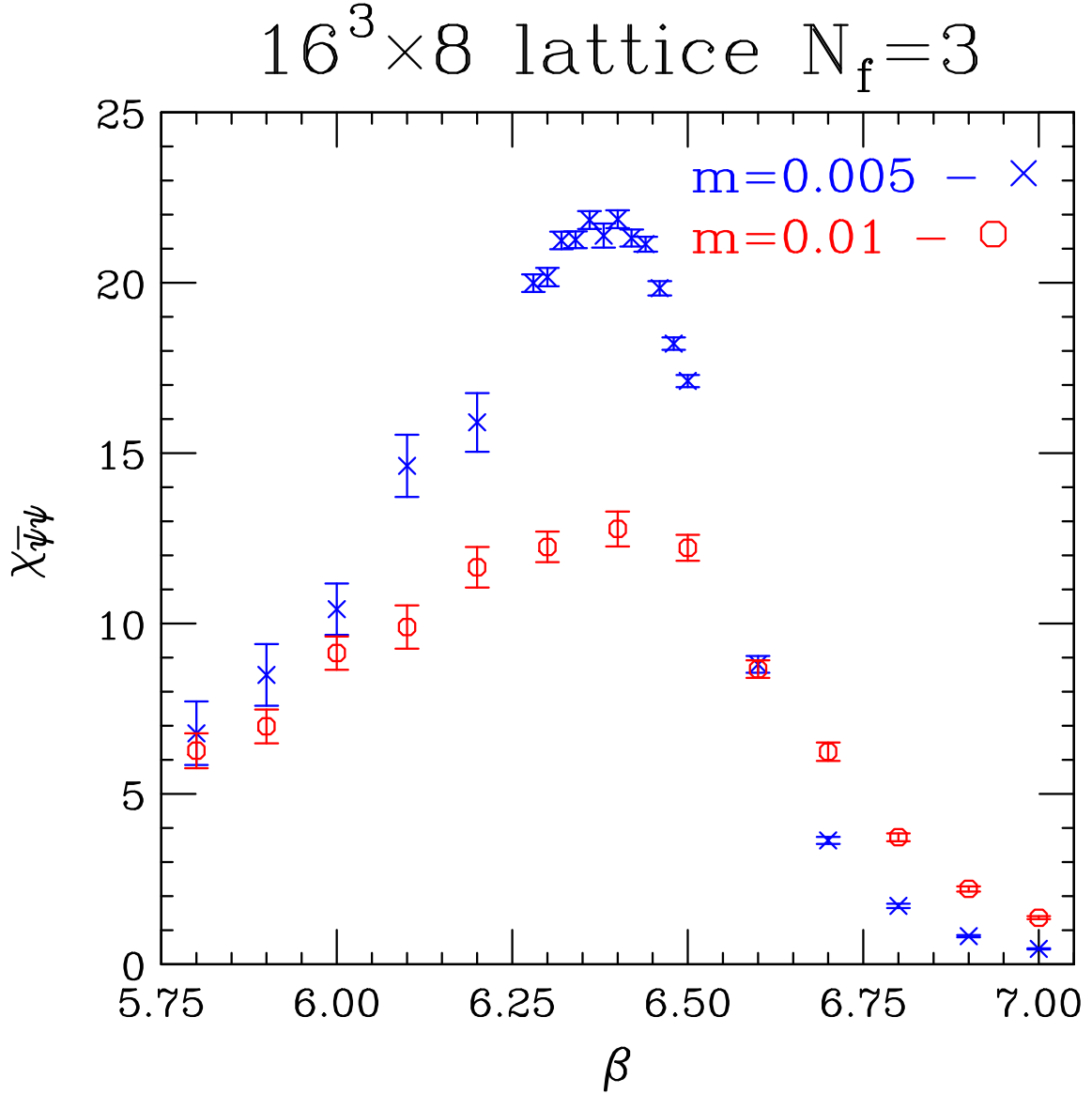


FIG. 5: Chiral susceptibilities as functions of $\beta = 6/g^2$ on a $16^3 \times 8$ lattice, in the state with a real positive Wilson Line, for $m = 0.01, 0.005$.

Figure 5 shows the (disconnected) chiral susceptibilities from our $16^3 \times 8$ simulations at $m = 0.005$ and $m = 0.01$. Both masses show peaks, and as expected, the peak at the lower mass is more pronounced. To make best use of the ‘data’ close to the transition, we again fit this to a parabola. Fitting over the range $6.28 \leq \beta \leq 6.5$ where each of the points represents 100,000 trajectories (actually 80,000, since we discard the first 20,000 for equilibration), we find the position of the peak to be at $\beta_{max} = 6.371(3)$, while the fit has $\chi^2/d.o.f. = 2.2$. This fit is plotted over the ‘data’ in figure 6. Not surprisingly, this fit is less stable than the fit to the $N_t = 6$ susceptibilities. Removing the point at $\beta = 6.28$ changes the peak to $\beta_{max} = 6.376(3)$ while improving the quality of the fit to $\chi^2/d.o.f. = 1.6$. We therefore give $\beta_{max} = 6.37(1)$ as our best fit. A fit to the $m = 0.01$ ‘data’ over the range $6.1 \leq \beta \leq 6.6$ yields $\beta_{max} = 6.34(2)$ with $\chi^2/d.o.f. = 2.5$. Removing the point at $\beta = 6.1$ moves the peak to $\beta_{max} = 6.36(2)$ with almost no change in $\chi^2/d.o.f.$. Again, we consider β_{max} at $m = 0.005$ as our best estimate of β_χ .

The increase in β_χ from $N_t = 6$ to $N_t = 8$ is thus:

$$\beta_\chi(N_t = 8) - \beta_\chi(N_t = 6) = 6.37(1) - 6.278(2) = 0.09(1) \quad (15)$$

This is to be compared with the increase from $N_t = 4$ to $N_t = 6$

$$\beta_\chi(N_t = 6) - \beta_\chi(N_t = 4) \sim 0.3 \quad (16)$$

If we were still in the same scaling regime, one might expect that

$$\frac{\beta_\chi(N_t = 8) - \beta_\chi(N_t = 6)}{\beta_\chi(N_t = 6) - \beta_\chi(N_t = 4)} \sim \frac{\ln(8/6)}{\ln(6/4)} \approx 0.71 \quad (17)$$

The fact that the increase from $N_t = 6$ to $N_t = 8$ is somewhat smaller indicates that we are emerging from the strong coupling domain. However, there is still no sign that β_χ is approaching the expected non-zero constant value, expected for a bulk transition. If, however, this 3-flavour theory is QCD-like, the 2-loop β -function would predict (equation 6)

$$\beta_\chi(N_t = 8) - \beta_\chi(N_t = 6) = 0.002 - 0.003 \quad (18)$$

which is much smaller than what is observed. It should be noted that the reason this is so small is that $\beta_\chi(N_t = 8)$ is still quite close to the second zero of the β -function. For this reason 2-loop perturbation theory should not be trusted. However, the 2-loop β -function never becomes very large, so that the maximum possible change in β_χ between $N_t = 6$ and

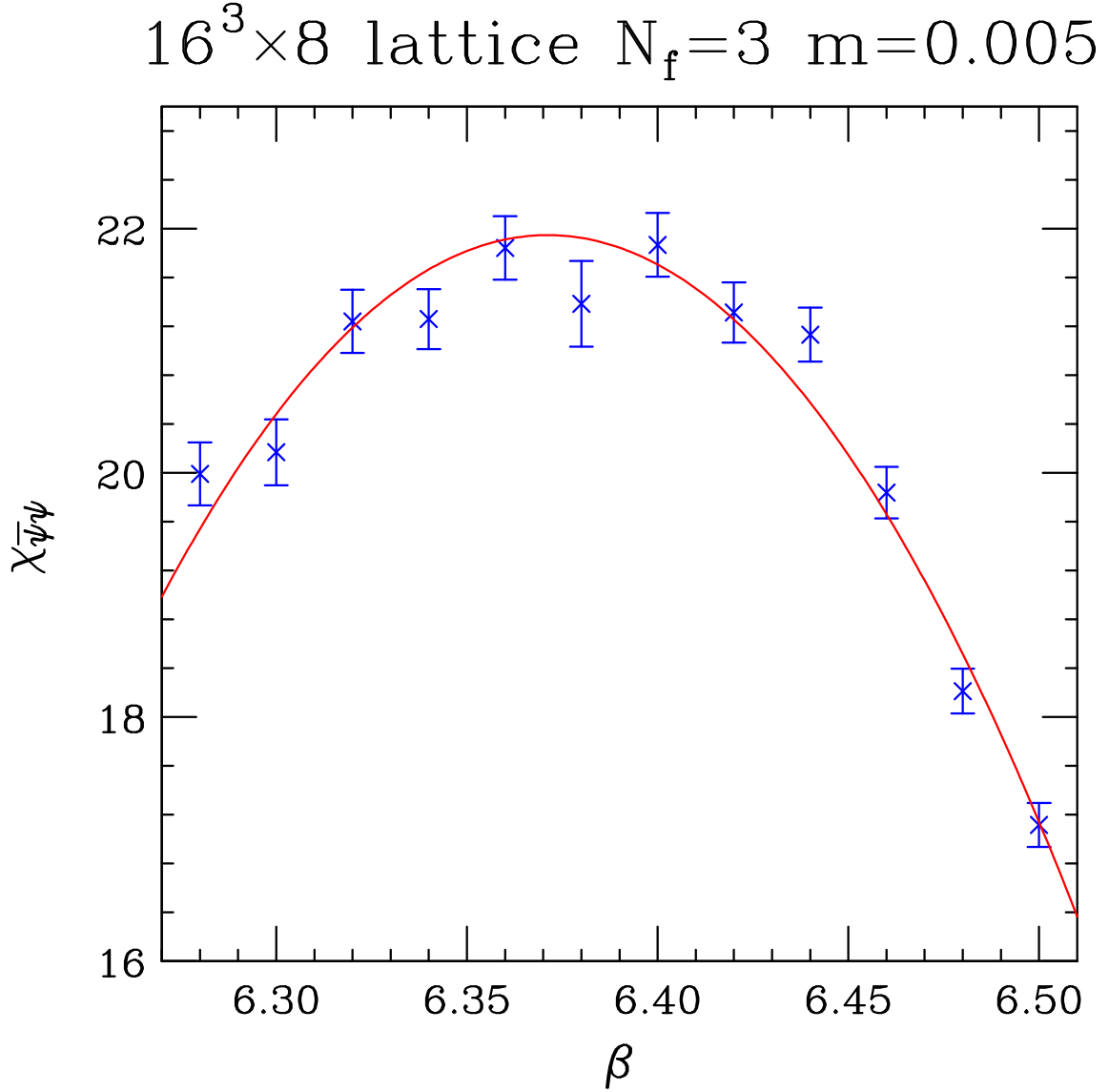


FIG. 6: Chiral susceptibility as a function of $\beta = 6/g^2$ on a $16^3 \times 8$ lattice, in the state with a real positive Wilson Line, for 0.005, showing the parabolic fit mentioned in the text.

$N_t = 8$, which it predicts, is only ≈ 0.022 . This bound is true to all orders, provided we are on the weak coupling side of all non-trivial minima of the β -function. Hence, although we have evidence of emergence from the strong-coupling domain, we are not yet able to access the large N_t limit.

IV. DISCUSSION AND CONCLUSIONS

We perform simulations of lattice QCD with 3 light colour-sextet quarks, to compare and contrast its behaviour with that of the 2-flavour version, a candidate walking-Technicolor theory. Finite-temperature simulations are performed at $N_t = 6$ and $N_t = 8$ to determine β_χ the coupling $\beta = 6/g^2$ at the chiral-symmetry restoration phase transitions. In particular we are looking for evidence that β_χ tends to a finite limit as $N_t \rightarrow \infty$, since it is expected that this theory is a conformal field theory, where the chiral transition is a bulk transition.

Our simulations show that between $N_t = 6$ and $N_t = 8$, β_χ increases by 0.09(1). Although this indicates that by $N_t = 8$, β_χ is no longer in the strong-coupling domain, it does not yet indicate that the chiral transition is a bulk phase transition. β_χ also fails to evolve as would be predicted by asymptotic freedom for a finite temperature transition. Hence we will need to perform simulations at larger N_t . (Simulations at $N_t = 12$ have been started.)

Table I gives the positions of the deconfinement transitions (β_d) and the chiral transitions (β_χ) for $N_t = 4, 6, 8$ from this and previous studies. (Here we note that, since we have only used a single spatial volume for each N_t , lack of significant finite volume corrections is only an assumption, based on previous experience, which suggests that $N_s = 2N_t$ is adequate.)

N_t	β_d	β_χ
4	5.275(10)	6.0(1)
6	5.375(10)	6.278(2)
8	5.45(10)	6.37(1)

TABLE I: $N_f = 3$ deconfinement and chiral transitions for $N_t = 4, 6, 8$. In each case we have attempted an extrapolation to the chiral limit.

In the simulations described in this paper, we have worked in the phase where the Wilson Line (Polyakov Loop) is real and positive. These Wilson Lines are large close to the chiral transitions, and show little if any indications of this transition.

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